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A Simple Scheme for Implementing Wave Absorption in Quasi-Neutral PIC Simulations of ECR Plasma

WALLACE M. MANHEIMER

Senior Scientist For Fundamental Plasma Processes
Plasma Physics Division

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A simple scheme is formulated here for describing the absorption of electron cyclotron waves in ECR plasma reactors. We particularly focus on quasi-neutral particle simulation schemes, where short times like the inverse electron plasma and cyclotron frequeencies are not resolved. The formulation here implements a wave kinetic equation for propagation along the magnetic field and the self consistent quasi-linear response of the electrons. The velocity dependence of the wave deposition is correctly described, maxwellian electrons are not assumed so the tail of the electron distribution can be either overpopulated or depopulated, depending on the dominant physical processes present. The computer time to solve the problem and the human time to code it up are both minimized.

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A SIMPLE SCHEME FOR IMPLEMENTING WAVE ABSORPTION IN QUASI-NEUTRAL PIC SIMULATIONS OF ECR PLASMA

I Introduction

Electron cyclotron resonance (ECR) plasma processing reactors are one of the earliest high electron density reactors to be considered[1], and still play an important role in semiconductor etching, particularly in the etching programs at NRL. Recent efforts in NRL Plasma Processing ARI (accelerated research initiative) modeling program have focused on the low pressure ECR reactor[2-4]. The basic dilemma in conventional modeling is that both the electron and ion species of the reactor have long mean free path so they are not fluid-like; however the plasma self electric fields are very important in determining the dynamics of the reactor. In this case, one would think a standard particle simulation would be the necessary computational tool to bring to bear. The difficulty is that the time step is then limited to a time less than the inverse electron plasma frequency (perhaps a few picoseconds), while the time scale of interest in the physics is the time to form the equilibrium, including the chemical equilibrium (hundreds of microseconds to milliseconds). The approach used was the development of a quasi-neutral particle simulation scheme, which maintains the full particle nature of the plasma, but avoids the electron plasma frequency time scale. The original application was to an ECR discharge. The main thing missing from the model developed so far[2] is a description of the propagation and absorption of the cyclotron waves. The models up to now have assumed only a simple electron acceleration scheme near the cyclotron resonant surface which is specified separately in essentially an ad hoc manner.

The electron cyclotron waves are launched through a waveguide and injected into the plasma through a quartz vacuum window. Once in the plasma, they propagate to the resonant surface where they are self-consistently absorbed by the plasma which the waves themselves create. In creating this plasma, they deposit their energy into the electrons in some energy dependent manner which we would also like to resolve. That is, we would like to solve not only for the proper plasma density (related to the absorbed power), but also for the electron distribution function which is consistent with the microwave damping and plasma production. Furthermore, so as keep the times scales consistent with those in the existing simulation, we would like to solve for this in a manner which does not introduce the electron cyclotron or electron plasma frequency time scales. This paper develops a formulation which accomplishes just that. The actual implementation in a simulation scheme will be addressed in a future work.

The NRL ECR reactor, and most others as well, have a magnetic field structure determined by several external coils. In almost every case, the magnetic field at the vacuum window is higher that that required for cyclotron resonance with the incoming waves. The magnetic field decreases as one moves away from this window, so as the waves propagate into the plasma, they approach the position of cyclotron resonance, at which point they deposit their energy. It is important to realize that there are two polarizations the wave might have as it propagates along the field. These are right circularly polarized, which is resonant with the electrons at cyclotron resonance, and left circularly polarized which is not resonant with the electrons. In the NRL source and many others, the input waveguide is a fundamental mode rectangular waveguide, so the

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electric field is linearly polarized. Thus both allowed circular polarizations enter the plasma with roughly the same amplitude. This seems to be a very important fact in explaining the qualitative nature of the wave propagation in the plasma. One might think that a circular waveguide input would be preferable. There the polarization could be controlled, and one could choose to inject only a right circularly polarized wave, the wave most easily absorbed. Although most ECR reactors do inject through rectangular waveguide, one recent series of experiments has injected circularly polarized microwaves through circular waveguide, and has seen simpler behavior.[5,6]

In the next section, we discuss the wave propagation as well as the qualitative nature of the observed microwave absorption and plasma production. In doing so, we also discuss other ECR reactors, how their results compare with those from NRL, and also the implications of all of these results for theory. We also briefly review other theoretical treatments of the problem. The remainder of this work formulates a theory of the propagation and absorption of the right hand circular wave in the plasma, the self consistent plasma response, and the way this formulation can be simply and economically included in the simulation scheme we have developed. As we will see, the theory is fully self consistent whether or not the electron distribution function is Maxwellian. Furthermore, depending on how one contours the magnetic field in space, the electron distribution function may or may not have a large nonthermal tail. In fact this ability to tailor the electron distribution function by adjusting the magnetic field profile may prove to be one important advantage of ECR reactors. Our formulation, coupled with the simulation codes[2-4] should be able to model this aspect of the plasma reasonably accurately. Thus the formulation we develop has all of the qualities enumerated earlier. It should make the calculation of plasma properties, as a function of injected power and microwave configuration, much more accurate. However the theory is formulated only for the right hand wave. The propagation of the left hand wave can be handled by a ray trace calculation in one or two dimensions, but this wave is not absorbed unless it is depolarized, for instance by reflection. Thus a quantitative description of the plasma including both polarizations would be much more complicated. However it is worth noting that ECR reactors can be run, have been run, and is probably preferably should be run with only the right hand circularly polarized wave initially injected.

II. Waves in the Cold Plasma, and Qualitative Nature of the Observations in the NRL ECR Reactor.

In the NRL ECR reactor, the waveguide connects to the outer edge of the vacuum chamber, separated from the waveguide by a quartz window, in such a way that the microwave propagation, both in the waveguide and in the plasma is mostly along the magnetic field. The microwave frequency is 2.45 GHz, so the magnetic field at cyclotron resonance is 875 G. A schematic of the NRL ECR reactor is shown in Fig.(1). Several magnetic field configurations are used, two of which are shown in Fig.(2). The first is called the standard profile, which has a uniformly decreasing field with a value higher than for cyclotron resonance at the window. The other field configuration is similar, but it has a lower magnetic field so that the cyclotron resonance position at the window. For field aligned propagation, the cold plasma dispersion relation allows for two modes of propagation, right hand circularly polarized with dispersion relation

$$n^2 \equiv \left(\frac{kc}{\omega}\right)^2 = 1 - \frac{\omega_e^{\,2}}{\omega(\omega - \Omega\cos\theta)} \qquad (1)$$

and left hand circularly polarized with dispersion relation

$$n^2 \equiv \left(\frac{kc}{\omega}\right)^2 = 1 - \frac{\omega_e^{\,2}}{\omega(\omega + \Omega\cos\theta)} \qquad (2)$$

Here ω_e is the electron plasma frequency, Ω is the electron cyclotron frequency, taken to be positive, and θ is the angle between the phase velocity of the wave and the magnetic field. Unless we are considering propagation away from the direction of the magnetic field, we take $\theta=0$.

Let us consider first the right hand circularly polarized wave. It has a resonance at $\omega = \Omega$, and a cutoff at $\Omega = (\omega^2 - \omega_e^{\,2})/\omega$. In the magnetic field configuration, the wave is injected below the cyclotron frequency and propagates into a decreasing magnetic field. As long as $\omega < \Omega$ at the point of injection, the wave will propagate at any plasma density; i.e. there is no maximum density for propagation. This is undoubtedly the reason ECR reactors are successful in generating plasmas with high ($\omega_e >> \Omega$) electron density. However just beyond the cyclotron resonance, there is of course no propagation. As one follows the magnetic field line beyond the resonance, as the magnetic field and density both decrease, and one again comes into a region of propagation after passing cutoff.

Now consider the left hand circularly polarized mode. This mode has no resonance. (It is resonant with the ions at much lower frequency.) It does have a cutoff at $\omega_e^{\,2} = \omega^2 + \omega\Omega$. If $\omega = \Omega$, then this plasma cutoff is at twice the critical density.

Let us now consider the ray paths of the left and right circularly polarized waves. The rays are oriented along the direction of the group velocity. We consider only the

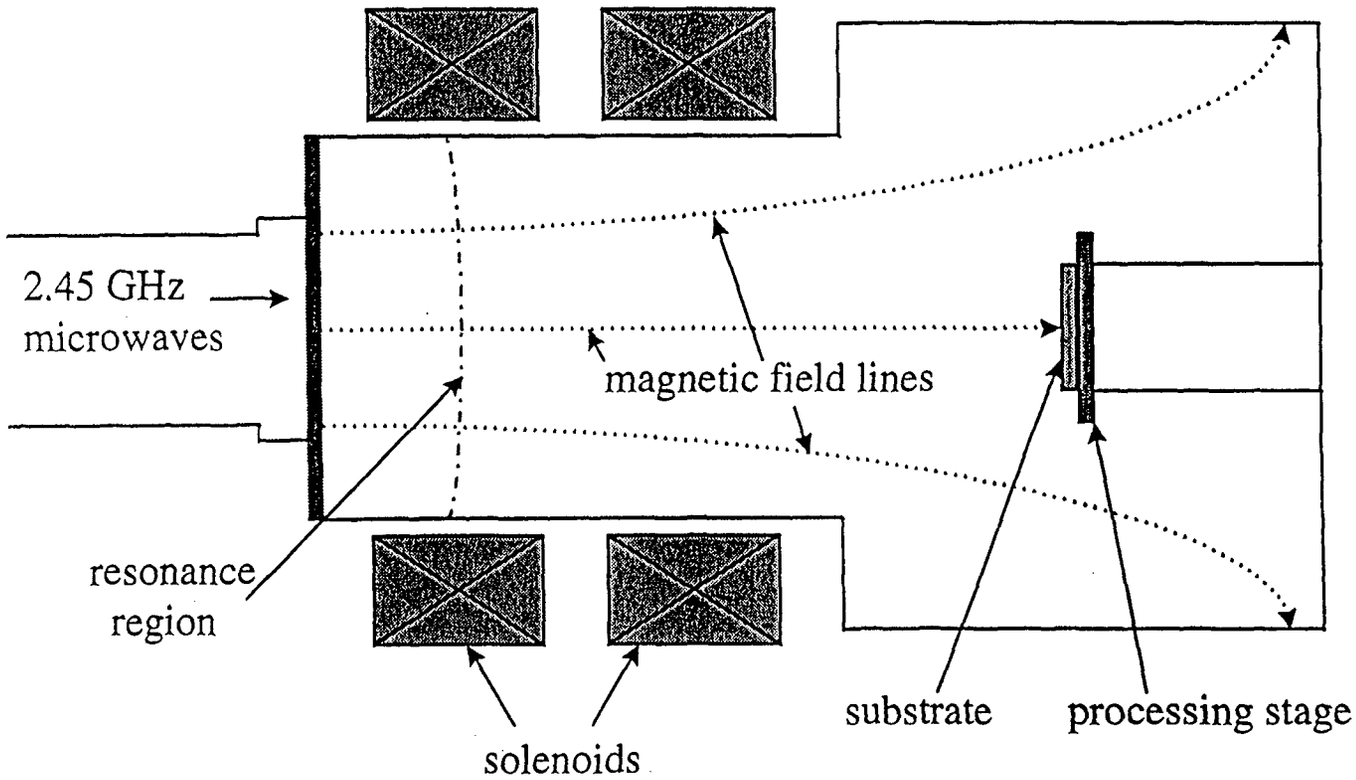

Fig. 1 — Schematic drawing of a typical two-magnet ECR plasma reactor.

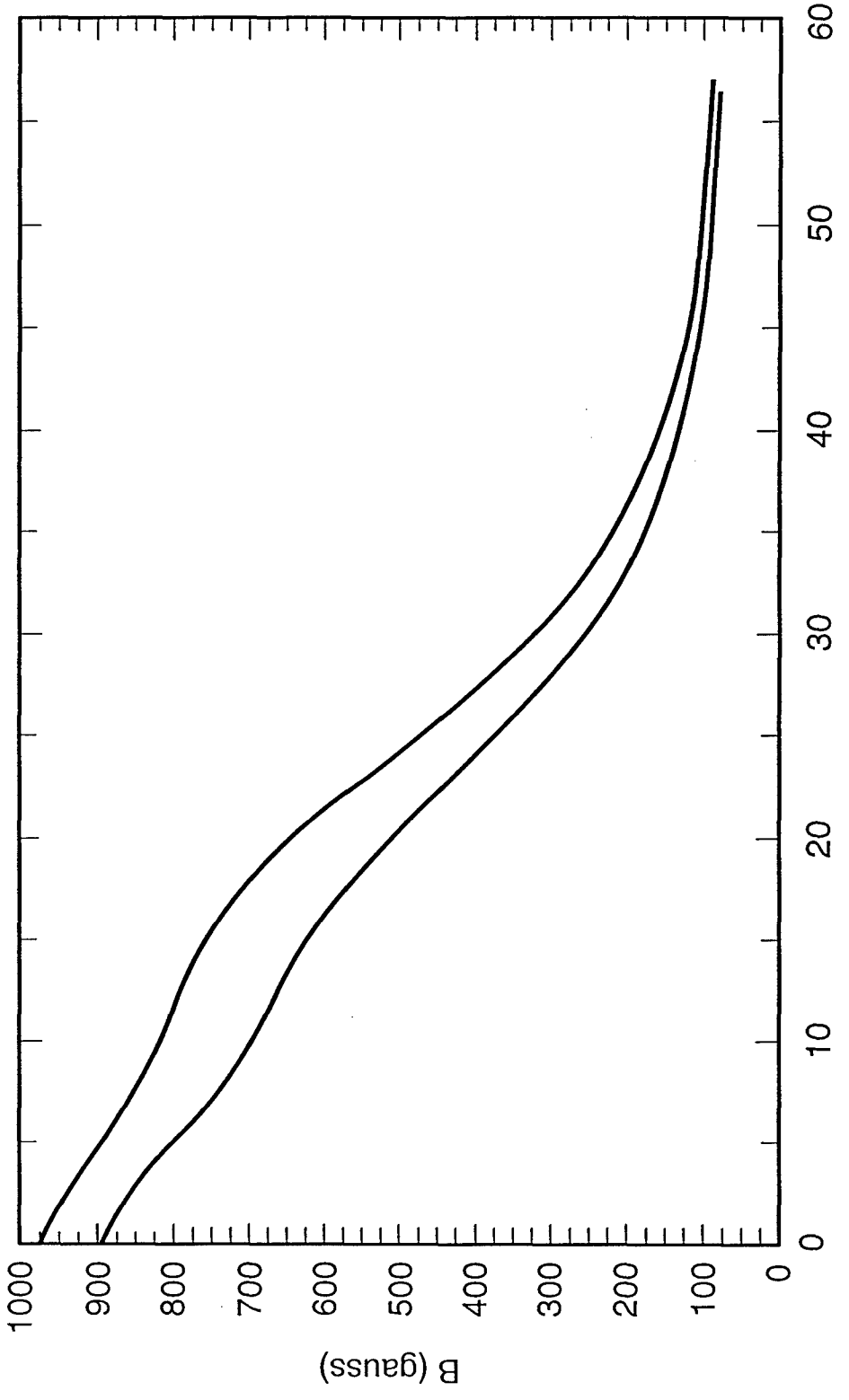

Fig. 2 – Two of the possible field configurations for the ECR plasma reactor.

right hand wave near resonance and the left hand wave near cutoff. For the right hand wave near resonance, the first term on the right hand side of Eq. (1) is negligible, and the dispersion relation for ω as a function of k becomes

$$\omega = \Omega \cos\theta \left[1 + \frac{\omega_e^{\,2}}{c^2 k^2} \right] \qquad (3)$$

Taking the gradient of ω with respect to k in spherical coordinates in k space, we find that the θ component of the group velocity, for small θ is approximately $-c^2 k\Omega\theta/\omega_e^{\,2}$. That is the group velocity is in the negative θ direction and is proportional to θ. Hence for small deviations of the phase velocity from the field line, the ray path tends to converge back to the field line. That is the microwave power tends to flow along the field lines to the point of electron cyclotron absorption. However, further from cyclotron resonance, another important effect is that the waves refract away from regions of high density[5,6]. Thus as the waves enter at high field and propagate toward lower field, they spread out for two reasons. First the magnetic field is divergent, and the waves tend to duct along the field; and second, the waves refract away from regions of high plasma density. For convenience, and to simplify the theoretical development, we do not consider the refraction here, although it is simple enough to include in the formulation with existing ray tracing codes.

Now consider the left hand circularly polarized wave near cutoff. If ω is near the cutoff frequency ω_o, let $\omega = \omega_o + \delta\omega$, and assume that both k and θ are small. In this case, one finds that for small θ, the θ component of the group velocity is in the positive θ direction and is proportional to θ. Thus near cutoff, the left hand polarized wave tends to bend away from the field line.

We now discuss qualitatively the nature of the observations on the NRL ECR reactor. As we have said, the waveguide configuration is such that waves near, but below the electron cyclotron frequency are launched parallel to the magnetic field from the high field side of the reactor. We assume also that there is a matching network so that there is no reflection directly from the vacuum window, and that reflections are from the plasma only.

One of the main observations is that the electron plasma density can be very high[7]. Langmuir probe and 140 GHz interferometry measurements show that the spatially averaged electron density is about 10^{12} cm^{-3} at maximum microwave power input (about 500 W). Even at rather low microwave power, the electron plasma density is over 10^{11} cm^{-3} on axis. Since the gas pressure is about 1 mtorr, the plasma can be as much as 3% ionized. Since the microwave frequency is 2.45 GHz, the electron density in the plasma can be more than an order of magnitude greater than the critical density at the injected frequency, which is about $6 \times 10^{10} cm^{-3}$. At all but the very lowest microwave power, the maximum electron density also is large compared to the cutoff density for the left hand mode.

Another striking observation in the NRL experiment is that for the standard field profile, there are two modes which have been called the high and low modes[7]. As the microwave power is increased, there is a rather abrupt transition. In all cases, the maximum electron density increases with input microwave power. However at some particular power, there is a step increase in electron density (perhaps by almost a factor of 2) as the power is raised. What is even more notable is that the reflection of the microwave power suddenly drops as the power increases above this threshold. A typical plot of average electron density from interferometry, and percent of reflection, as a function of microwave power is shown in Fig. (3) for the NRL ECR reactor[7]. Here the fill density is 1 mtorr and the gas is argon. It can also be seen from Fig. (3) that at the highest injected power, the reflection begins to rise again and the electron density begins to fall. However this effect is not nearly as dramatic as the low to high mode transition.

The high and low modes have also appeared in other work on ECR plasmas[8-10]. In these works however, the behavior is somewhat different. For their cases of monotonically decreasing magnetic field, i.e., no magnetic mirror, Carl et al[8] see an abrupt transition at an input power of about 40 Watts. Crossing this transition, the electron density at the probe position jumps by about an order of magnitude, from about $3x10^{10}$ cm^{-3} to about $3x10^{11}$ cm^{-3}, and the reflected power also drops upon entering the high mode. Popov's experiments[9,10] show large reflection and transmission for electron densities below about $5x10^{10}$ cm^{-3}, and almost complete absorption for electron densities above about $7x10^{10}$ cm^{-3}. While Fig. (3) may show a glitch at the microwave power and electron density observed in Refs. (8-10), the main transition is at higher power and higher electron density.

It might be tempting to attribute this transition to the tunneling of the right hand circularly polarized wave through the cyclotron resonance, to the cutoff and its emergence out the other side. As the electron density increases, tunneling decreases, and the absorption at the cyclotron resonance approaches 100%. Figure 4 shows the relative axial profile of microwave power along the axis[7], in the NRL experiment, for an incident power of 375 Watts. The microwave power goes to zero beyond resonance, consistent with the absence of tunneling. However the Budden tunneling formula predicts essentially 100% absorption at the plasma density generated, even at the lowest microwave power. Thus tunneling does not seem to be the explanation for the high mode to low mode transition. Carl et al[8] also note that Budden tunneling is not even consistent with their data, which shows a transition at much lower electron density.

What is more likely in the NRL experiment is that at lowest density, the left hand mode propagates back and forth through the vacuum chamber, and ultimately all of part of it is reflected back through the input waveguide. At the lowest power and electron density, microwave power is seen on axis beyond the cyclotron resonance[7]. This is almost surely the left hand wave. At the higher electron densities, this wave becomes cutoff on the axis, although it may propagate in the outer radial regions. There they could convert to extraordinary modes (propagating mostly radially) and be absorbed at the

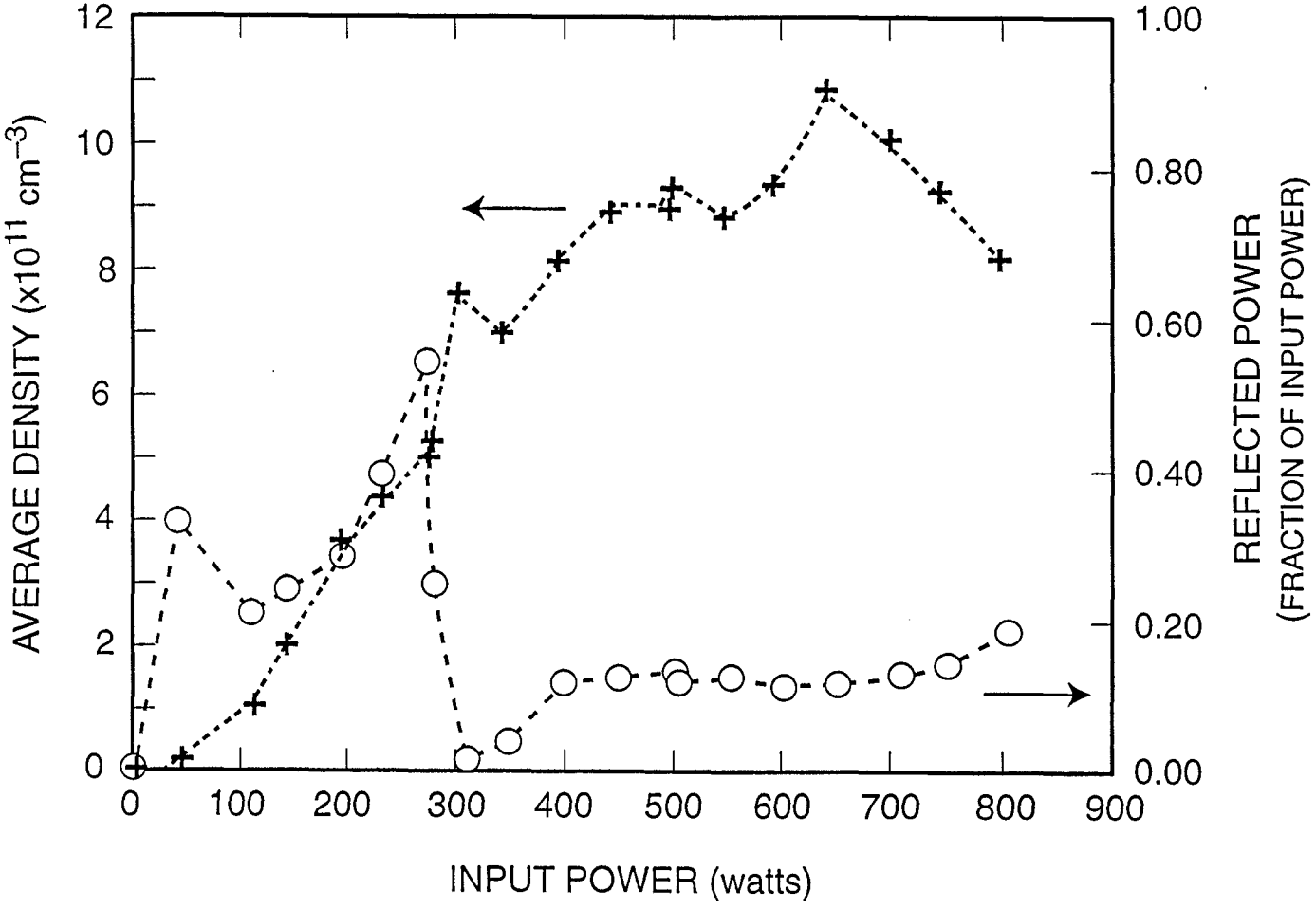

Fig. 3 – Electron density and microwave reflectivity vs incident microwave power.

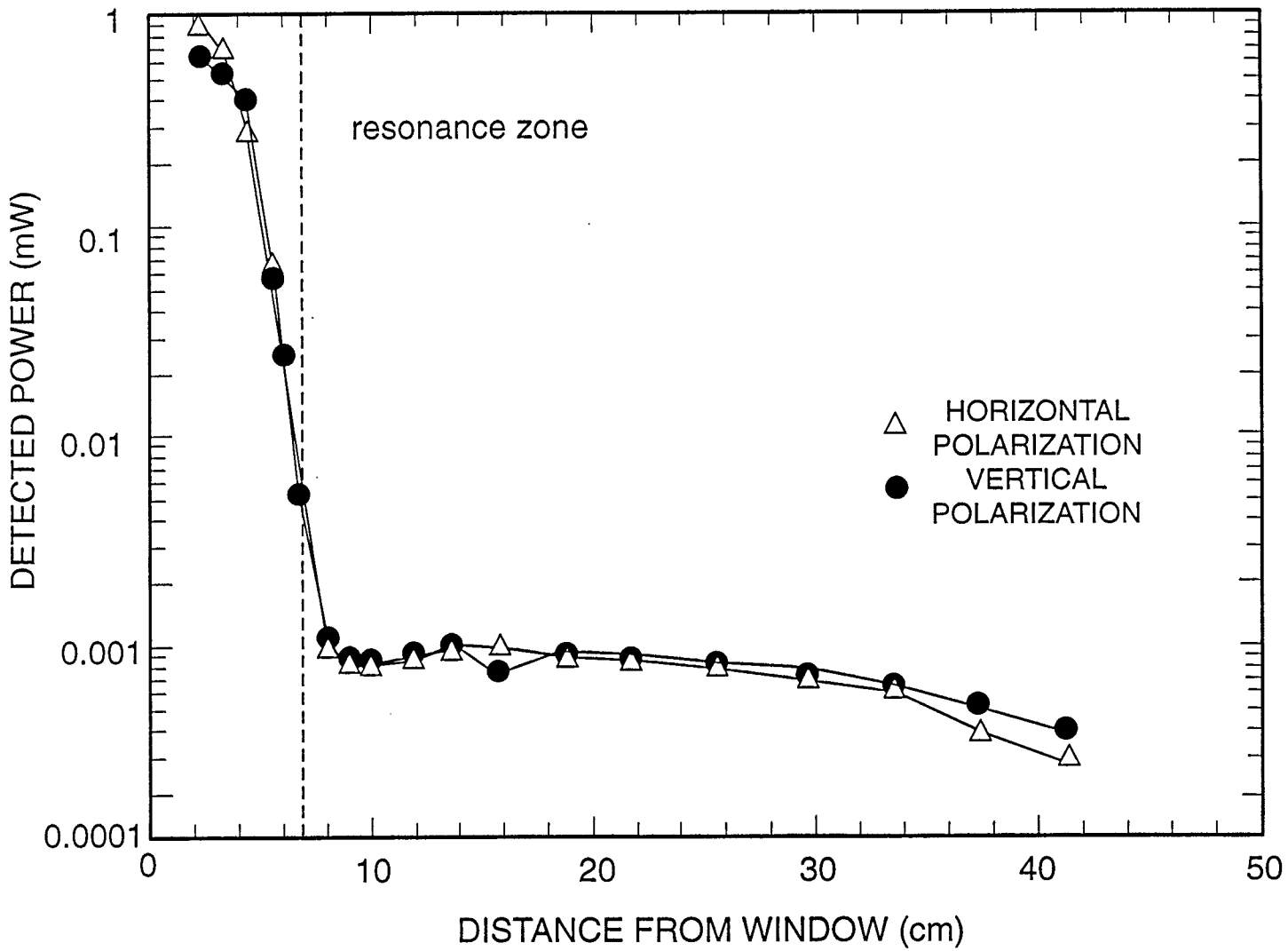

Fig. 4 – Relative microwave power on axis vs distance from window

upper hybrid resonance, $\omega^2=\omega_e^2+\Omega^2$. The ray paths do refract to the outer regions near cutoff as we have seen, although in the ECR reactors, the scale lengths are not long compared to the cutoff left hand mode wave length. Alternatively the left hand wave may be absorbed be absorbed in some sort of cyclotron resonance of a surface wave near the waveguide window. In any case, the low to high mode transition in the NRL ECR reactor seems to involve the left hand mode in some way, and the details appear to be rather complicated.

It is interesting that Ueda and Kawai[11] have observed extraordinary mode propagation in the outer radial region of an ECR plasma,. However they observed this mode only for a central density below about $2x10^{11}$ cm^{-3}, which is a rather low density compared to the NRL experiment. Nevertheless at low density this left hand mode probably gets into the plasma, converts to an extraordinary mode, and is absorbed or partially absorbed in the outer radial regions of the plasma at the upper hybrid resonance. According to this picture, as the injected power further increases, the electron density at the microwave window rises to where it is above the cutoff density for the left hand mode everywhere on the window. At this point the left hand mode could not get into the plasma and it would be reflected and perhaps also partially absorbed by a surface wave at the window. This could be a qualitative explanation for the decrease in electron density and increase in reflection at the highest power.

Let us briefly review the treatment of the left hand polarized wave by previous authors. References 5 and 6 ignore it completely. Since they inject through circular waveguide, they usually inject only a right hand polarized mode, in which case this assumption is valid. However in some of their experiments they mix a TE_{11} mode with a TM_{01} mode, so that in these experiments, one would expect a left hand mode to be injected as well. Reference 8 seems to briefly mention the left hand wave and then dismiss it. References 9 and 10 also briefly mention it, but then say, citing Musil and Zacek[12], that that is absorbed at the resonant surface, where $\omega=\omega_e$ due to the transverse component of wave number. According to Ref. 12, the perpendicular wave number induces a resonance near the plasma frequency, and at this point, there can be coupling between the right and left hand waves. However, while a left hand mode may convert to a right hand mode and be absorbed, a right hand mode may also convert to a left hand mode and thereby *not* be absorbed. Thus it is not obvious that this resonance can increase the *total* absorption. Furthermore, if the electron density at the window is above the critical density, this coupling would not occur[12]. Thus the following qualitative picture emerges for waves with non-zero perpendicular wave number. If the electron density at the window is below the critical density, both modes enter the plasma, but there is a mode conversion point, and therefore energy exchange between the left and right hand modes at the point before cyclotron resonance where $\omega=\omega_e$. If the electron density at the window is between the critical density and the cutoff density for the left hand wave, both waves propagate into the plasma as cold plasma theory would predict, except that the wave length of the left hand mode is long enough that one must doubt the accuracy of a ray trace calculation for it. If the electron density at the window is above left hand mode

cutoff density, then the left hand mode is either reflected at the window, or partially absorbed in a surface mode.

It is also worth pointing out that in a carefully diagnosed experiment, Scharer et al[13] conclude that for high electron density, WKB theory for parallel propagating modes is reasonably accurate and there is little effect of transverse wave number on the propagation. Thus all authors, including this one, basically brush aside the effect of the left hand wave. However it is probably playing an important, though subsidiary role in all of the experiments except those of Refs. 5 and 6.

As is apparent from Fig. (4), the NRL experiment shows that 99% of the microwave power is absorbed before the cyclotron resonance point. This is also consistent with many of the other cited experiments as well. Thus these observations are not consistent with a model of simple deposition of microwave power at the resonant surface.

The disappearance of microwave power beyond the cyclotron resonance point shown in Fig. (4) may be consistent with the presence of left polarized modes, because on the axis, the electron density is greater than the left hand mode cutoff density almost everywhere, so one would not expect to see the left hand mode on axis. This hypothesis of the importance of the left hand mode in the low to high mode transition could be tested theoretically by doing a ray trace of the this mode as a function of electron density and electron density profile. Alternatively, it could be tested experimentally in one of two ways. The first is by launching the wave into the chamber through a circular waveguide whose polarization could be controlled by the input structure as in Refs. 5 and 6. The second is to look for microwave power at large radius in the existing experiment.

Another experimental observation is the 'blue core' mode[7]. For the standard field profile, the position of cyclotron resonance is about 7 cm from the waveguide flange. In this case, it may be true that the left hand mode can refract around the maximum electron density and propagate in the outer radial region of the plasma. However if the current in the magnetic field coils are adjusted so that the position of cyclotron resonance is just at the flange, then the discharge takes the form of the 'blue core' mode. Here, the entire discharge is more constricted than that of the 'high mode'. Also the discharge is visibly different. The waveguide opening is visible as a blue core, with a faint pink corona around it, and it is likely that the discharge exists only along the those field lines which project back close to the waveguide opening. It seems that the probable explanation of this phenomenon is that if the cyclotron resonance position is at the waveguide flange, the right hand mode is immediately absorbed with no opportunity to refract out radially, and as long as the electron density there is above about 10^{11} cm^{-3}, the left hand cannot propagate at all in the plasma. It must either be reflected and/or absorbed by surface fields at the window. As we will see, the way in which the microwave deposits its power in the electron distribution function can depend sensitively on the magnetic field profile near the absorption position. Thus the standard and blue core modes may have rather different electron distribution functions (with the blue core mode being less likely to have

a non thermal tail on the electron distribution function). This then may account for their different optical properties.

To summarize, it seems very likely that in the NRL and other experiments, both the left and right circularly polarized waves are playing an important role in the physics of the device. However the propagation and absorption of the left hand wave is very complex and has not been adequately treated for a thermal plasma in any of the theoretical models to date. If only the right hand wave were present, the behavior of the reactor would probably be clearer and more predictable. One could most likely optimize performance of the reactor in parameter space more reliably and predictably if only this mode were present. Therefore, in this work, we present the self consistent theory of the propagation and absorption of right hand wave in a way in which it can be easily and economically incorporated into the NRL quasi-neutral particle simulation.

III Propagation and Damping of the Right Hand Cyclotron Wave.

We now turn to the development of the theoretical formulation, and also review some of the other published theoretical work. Our formulation assumes propagation from some starting point to cyclotron resonance. The basis of our calculation is a WKB calculation of wave propagation along a field line, together with the damping and the self consistent plasma heating. Specifically it is *not* necessary to assume that the electron distribution function is Maxwellian. The wave damping is determined from the exact distribution function which can be determined from the simulation[2-4] , and the plasma heating and wave damping is consistent with this.

There are many reasons the distribution function may be non Maxwellian. Ionization and excitation naturally deplete the tail. On the other hand, the heating process may give rise to a non thermal tail. To see this, note that cyclotron damping energizes particles with parallel velocity equal to $(\Omega-\omega)/k$. Depending on the spatial dependence of $\Omega(z)$, there may a large region of the plasma where the resonant velocity is high. Then the wave would damp out almost completely before the resonant velocity reached into the thermal part of the distribution function. On the other hand, if $\Omega(z)= \omega$ at the waveguide window (or else approaches it very abruptly in space), the heating will be in the thermal particles. This could be one possible explanation of the differences between the high mode and the 'blue core mode' in the NRL experiment. For the standard field profile, the distribution function may be generated with a non thermal tail because the cyclotron wave damps out further from cyclotron resonance, where the energetic particles are resonant. However for the 'blue core mode', the absorption must be by the thermal particles, since the resonant position is at or very close to the window. Thus, while the two plasmas absorb about the same power and have about the same electron density and temperature, the distribution functions generated may be different, implying different chemistry and excitations (i.e. visible color).

Thus by appropriately contouring the field, an ECR reactor allows some flexibility in the type of electron distribution produced. This could be a very great advantage of ECR reactors as compared to other types of high electron density reactors. With the simulation schemes developed[2-4], and the wave deposition model developed here, this can most likely be modeled with reasonable accuracy.

References 5 and 6 treat the problem most like we do here, except in their calculation of damping the plasma is assumed to be Maxwellian. Their model for the plasma is a simple diffusion equation which is coupled to their equation for wave deposition. Williamson et al[14], in a one dimensional treatment consider Budden tunneling of the right hand mode in realistic density and field profiles. Their results appear to be most important for fairly low density plasmas, $\omega_p \approx \Omega$. Ashtiani et al[15] develop a simulation code rather like ours, but assume power is deposited at the cyclotron resonance. They also consider cyclotron damping away from resonance, but the power lost by the wave in this cyclotron damping does not appear to be deposited in the plasma. Also they assume damping based on a Maxwellian distribution function. A very

interesting calculation is that by Yasaka et al.[16] They solve the two dimensional full wave problem of wave propagation in a cold, weakly collisional plasma with no assumption regarding polarization. The calculation assumes a frequency ω but solves spatially in r and z. An antenna is assumed to drive the system, and depending on where the antenna is, the propagation may be mostly axial or mostly radial. The calculated absorption (from collision absorption in a cold plasma) then goes into ionization, and the electron density is calculated from a dimple diffusion equation. Reference 16 probably gives the greatest degree of realism as regards geometry and polarization, that one can achieve economically (i.e. without a full fast time scale particle simulation). On the other hand, it seems that the formalism developed here, coupled ot the simulations of Ref. 2-4 will give the greatest degree of 'thermal' realism that one can achieve economically.

We now proceed with the development of the formulation. For propagation along the field line, the dispersion relation of the right hand circularly polarized wave is given by

$$n^2 = 1 - \frac{\omega_e^{\,2}}{\omega(\omega - \Omega)} \qquad (4)$$

and one can calculate that the group velocity along the magnetic field is given by

$$\frac{d\omega}{dk} = \frac{2kc^2(\omega - \Omega)^2}{\omega_e^{\,2}\Omega} \qquad (5)$$

The wave enters the plasma at a frequency near but below the electron cyclotron frequency, and propagates along the field toward lower magnetic field. As the wave approaches the cyclotron resonance, k approaches infinity as $(\Omega-\omega)^{-1/2}$, so the group velocity approaches zero at this point at $(\Omega-\omega)^{3/2}$.

Now let us consider the wave energy density. It is given by

$$W = \frac{E^2}{16\pi}\omega\frac{\partial}{\partial\omega}\left[1 - \left(\frac{kc}{\omega}\right)^2 - \frac{\omega_e^{\,2}}{\omega(\omega-\Omega)}\right] \approx \frac{E^2}{16\pi}\frac{\omega_e^{\,2}\Omega}{\omega(\Omega-\omega)^2} \qquad (6)$$

where E is the amplitude of the electric field and we have assumed high electron density in writing the right hand side of Eq. (6). The power density flux of the wave is the group velocity times the energy density

$$\mathbf{P} = \mathbf{v_g} W \qquad (7)$$

and the wave kinetic equation is

$$\frac{\partial W}{\partial t} + \nabla \bullet \mathbf{P} = -2\gamma W \qquad (8)$$

where $-\gamma$ is the cyclotron damping rate of the wave. We consider two approximations for the ray path. As we have seen in the last section, the ray paths of the cyclotron waves tend to bend into the field line, so the simplest approximation is to consider only propagation along the magnetic field. The other approximation is to use the actual ray path, where a unit vector along the ray is denoted $\mathbf{i}_{ray}(s)$ where s is the distance along the ray path (which may be the actual ray path, or for simplicity may be approximated as the field line. Thus we may make the approximation

$$\mathbf{v}_g = v_g \mathbf{B}/B \qquad (9a)$$

or more accurately,

$$\mathbf{v}_g = v_g \mathbf{i}_{ray} \qquad (9b)$$

and assume there is no time dependence to the ray equation. Then taking the divergence, and making use of the fact that the magnetic field itself has zero divergence, we find that the ray trace equation for the electron cyclotron wave is

$$\frac{\partial}{\partial s}\left[\frac{v_g W}{B}\right] = -\frac{2\gamma W}{B} \qquad (10a)$$

or more accurately,

$$\nabla \bullet v_g W \mathbf{i}_{ray} = -2\gamma W \qquad (10b)$$

where s is a measure of distance along the magnetic field. For each magnetic field line, Eq. (10A) is a one dimensional equation along that line. Equation (10B) is also a one dimensional equation, but now along the actual ray path. For the purpose of this paper, we usually use the simpler approximations of the ray path being the field line. However in actual implementation, where refraction may be important in spreading out the wave power away from the field lines it started on, the B equations would more likely be used. Notice that even though the wave propagates nearly parallel to the field line, small deviations from parallel propagation can take the ray far from the original field line over long propagation distances. Thus to consider the spreading of the wave energy away from the field lines projecting back to the waveguide opening, it is necessary to consider refraction, that is the B equations.

For the approximate solution, the A equations, the ray trace equation has a particularly simple form. It is just a single equation for each field line. In the quasi-neutral simulations of the ECR reactor, there is already an equation for the electron dynamics along the magnetic field. Thus it is a simple matter to add one additional

equation along each field line to describe the ray propagation. For a more accurate ray trace, we would use the B equations.

We now have to work out an expression for the cyclotron wave damping γ. To calculate this, we rely on the description of cyclotron wave damping in Stix[17]. The equation for the electric field **E**, which determines the dispersion relation is

$$\mathbf{k} \times \mathbf{k} \times \mathbf{E} + (\omega/c)^2 \in \bullet \mathbf{E} = 0 \qquad (11)$$

where $\in$ is the dielectric tensor, given by $\in = \mathbf{I} + \chi(\omega,\mathbf{k})$, and χ is given by Stix as

$$\chi = \left(\frac{\omega_e^{\,2}}{\omega\Omega}\right)\int d^3p \left[\begin{array}{l} \mathbf{I}\left(\frac{\Omega p_\perp}{2\omega}\right)\frac{\partial f}{\partial p_\perp} + \mathbf{e}_z\mathbf{e}_z\left(\frac{\Omega}{2\omega}\right)\left(2p_z\frac{\partial f}{\partial p_z} - p_\perp\frac{\partial f}{\partial p_\perp}\right) \\ +(\Omega p_\perp)\left[\left(\frac{kp_\perp}{m\omega}\right)\frac{\partial f}{\partial p_z} + \left(\frac{\Omega}{\omega}\right)\frac{\partial f}{\partial p_\perp}\right]\frac{\mathbf{T}}{\omega - kv_z - \Omega} \end{array}\right] \qquad (12)$$

where have assumed $\omega \approx \Omega$ and have neglected the effect of the cyclotron harmonics. **T** is a complicated tensor defined by Stix, involving Bessel functions. Here f is normalized so that its integral over a three dimensional momentum space is unity. We approximate the damping by assuming here that the wave propagates only along the field line, i.e. $k_\perp = 0$. Thus the only effect of $k_\perp \neq 0$ we consider is the fact that a wave may separate from the field line it started on. Otherwise we neglect the effect of $k_\perp \neq 0$. In this case, the tensor **T** simplifies considerably

$$\mathbf{T} = \begin{bmatrix} \frac{1}{4} & \frac{i}{4} & 0 \\ -\frac{i}{4} & \frac{1}{4} & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad (13)$$

To continue, we will make one further approximation as regards the system. The particle simulation for the electrons is executed by following their motion along the field and also by keeping track of their magnetic moment as it changes due to collisions. Since in practice, the collisions isotropize the electron distribution function rather quickly, we will assume that the electron distribution function is isotropic in momentum space, so that it depends only on the magnitude of the momentum variable, p. Then, one can write out the expression for χ as an integral in momentum space in polar coordinates, p and θ, where θ is the momentum space polar angle. It is

$$\chi = \left(\frac{\omega_e^{\,2}}{\omega\Omega}\right)\int d^3p \left[\begin{array}{l} \mathbf{I}\left(\dfrac{\Omega p \sin^2\theta}{2\omega}\right)\dfrac{\partial f}{\partial p} + \\ \dfrac{\mathbf{T}\Omega p \sin^2\theta}{4}\left\{\dfrac{1}{\omega - kv\cos\theta - \Omega} - \dfrac{1}{\omega}\right\}\dfrac{\partial f}{\partial p} \end{array}\right] \qquad (14)$$

where now **I** and **T** are 2x2 matrices in the transverse plane. It is not difficult to show that for a cold plasma, one can recover the dispersion relation for the right hand circularly polarized wave. (For the left hand circularly polarized wave one would also have to include denominators going as $(\omega+\Omega)^{-1}$.)

To recover the damping rate of the electron cyclotron wave, we take the residue part of the singular denominator in Eq. (14)

$$\frac{1}{\dfrac{\omega-\Omega}{kv} - \cos\theta} = \pi i \delta\left(\frac{\omega-\Omega}{kv} - \cos\theta\right) \qquad (15)$$

Then one can write out the dispersion relation including the electron cyclotron damping as

$$\begin{array}{l} -k^2 + \left(\dfrac{\omega}{c}\right)^2 - \dfrac{\omega_e^{\,2}\omega}{c^2(\omega-\Omega)} + \\ \dfrac{\omega_e^{\,2}\pi^2 i\omega}{2\Omega c^2}\displaystyle\int_{p_m}^{\infty} p^2 dp\left(\frac{m\Omega}{k}\right)\left[1 - \frac{p_m^{\,2}}{p^2}\right]\frac{\partial f}{\partial p} = 0 \end{array} \qquad (16)$$

where $p_m = m(\Omega-\omega)/k$. The damping rate, $-\gamma$ is then given by

$$-\gamma = \frac{\pi^2(\Omega-\omega)^2\omega}{8\Omega^2}\int_{p_m}^{\infty} p^2 dp\left(\frac{m\Omega}{k}\right)\left[1 - \frac{p_m^{\,2}}{p^2}\right]\frac{\partial f}{\partial p} = 0 \qquad (17)$$

To implement this damping rate in the evaluation of Eq.(17), we must calculate f(p). This information is available from the particle simulation of the electron dynamics. Thus this expression gives us a damping rate which is self consistent with the electron dynamics as calculated from the particle simulation. Specifically, it is valid whether or not the electron distribution function is Maxwellian. For cases where the high energy electron tail is over populated (for instance due to the cyclotron heating), or depleted (for instance

due to ionization or excitation), the expression for the damping rate in Eq.(17) will still be consistent with the electron distribution function which is generated. Notice that for a distribution function which is a monotonically decreasing function of energy, $\partial f/\partial p < 0$, so that the wave damps. As we approach cyclotron resonance, this damping scales roughly as

$$\gamma \propto \frac{(\Omega-\omega)^2\omega}{\Omega k v_e} \qquad (18)$$

where v_e is the electron thermal velocity, and using the expression for the group velocity,

$$\frac{\gamma}{v_g} \propto \frac{\omega_e^2\omega}{(kc)^2 v_e} \propto \frac{(\Omega-\omega)}{v_e} \qquad (19)$$

where in the last relationship on the right side of Eq. (19) we used the fact that near resonance $(kc)^2 \approx \omega_e^2\omega/(\Omega-\omega)$. However, for significant damping, we must have $\Omega-\omega \propto kv_e$, so as the ray approaches the cyclotron resonant surface, the spatial damping rate is about equal to the wave number.

IV The Response of the Electron Distribution Function and a Proof of Self Consistency.

As the cyclotron wave damps, the electrons gain energy and are stochastically heated. We use the quasi-linear theory to model the electron response to the to the waves[18]. The quasi-linear equation for the response of the electron distribution function is

$$\frac{\partial f}{\partial t} = \left[\frac{\pi e^2 E^2}{32}\right]\left\{\left(1-\frac{kv_z}{\omega}\right)p_\perp{}^{-1}\frac{\partial}{\partial p_\perp}+\left(\frac{k}{m\omega}\right)\frac{\partial}{\partial p_z}\right\} \\ \delta(\omega - kv_z - \Omega)\left\{\left(1-\frac{kv_z}{\omega}\right)\frac{\partial}{\partial p_\perp}+\left(\frac{kv_\perp}{\omega}\right)\frac{\partial}{\partial p_z}\right\} f \qquad (20)$$

where the difference between the coefficients in front of Eq. (20) above and Eq. (17.41) of Stix is a result of the different normalization of the electric field (i.e. exponential notation vs. sine and cosine, including polarization etc.) Also the propagation is assumed to be entirely parallel to the magnetic field. What we would like to show now is that the expression for the damping of the electron cyclotron wave, derived in the last section is consistent with the energy gain of the electrons from quasi-linear diffusion, which is

$$\varepsilon' = \int d^3p\, (p_\perp{}^2/2m + p_z{}^2/2m)\, \partial f/\partial t \qquad (21)$$

Substituting from Eq.(20) into Eq. (21), it is simplest to calculate this by first integrating by parts over $p_\perp$ and p_z. Then the subsequent integrals are done in spherical coordinates in momentum space. Of course, as is consistent with the calculation in the previous section, we assume that the distribution function depends only on p and not on polar angle θ. Doing this, we find

$$\varepsilon' = -\left(\frac{\pi m \omega_e{}^2 E^2}{32k}\right)\int_{p_m}^{\infty} p^2 dp\left[1-\frac{p_m{}^2}{p^2}\right]\frac{\partial f}{\partial p} \qquad (22)$$

Using the expression for the wave energy density, Eq.(6), and the damping rate, Eq.(17), it is not difficult to show that the two results are consistent with one another, that is

$$2\gamma W = \varepsilon' \qquad (23)$$

Thus one way to self consistently simulate the response of the electrons to wave damping is to incorporate quasi-linear diffusion into the electron equation of motion.

V. Implementation in a Particle Simulation

We have seen that the electron cyclotron waves propagate along ray surfaces, which we may approximate as magnetic field lines, toward the low field regions. As they do, they damp, and the self consistent response of the particles is to diffuse in velocity space. As Stix points out[18], this diffusion obeys an additional constraint. As the particles diffuse, the change in perpendicular velocity is related to the change in parallel velocity in such a way that the particles are constrained to move along circles in v_z $v_\perp$ phase space which are centered at $v_z = \omega/k$. One can show this either by calculating the characteristics of the quasi-linear diffusion equation, Eq. (20), or by using the fact that as the particles diffuse in velocity space, energy and parallel momentum are conserved between waves and particles. (The parallel momentum density of the wave is (k/ω) times the parallel energy density.) Therefore if the change in parallel velocity, δv_z, is known, the change in perpendicular velocity is simply given by

$$\delta v_\perp = -[v_z - (\omega/k)]\delta v_z / v_\perp \qquad (24)$$

The parallel velocity is especially easy to work with because it is a Cartesian component. Considering only the parallel velocity, the quasi-linear diffusion equation (actually a Fokker- Planck equation) is

$$\frac{\partial f}{\partial t} = \left[\frac{\pi e^2 E^2}{32}\right]\frac{\partial}{\partial p_z}\delta(\omega - kv_z - \Omega)\left(\frac{kv_\perp}{\omega}\right)^2 \frac{\partial f}{\partial p_z} \qquad (25)$$

which represents a velocity space diffusion and dynamic friction. The idea is then to replace the Fokker Planck equation with the appropriate terms in a Langevin equation, which are then added to the other terms in the parallel electron equation of motion solved in the simulation.

The diffusion equation has a delta function in it, and this must be integrated in any finite difference treatment. For the case of cyclotron wave propagation, all rays have frequency ω, but the magnetic field, and therefore the wave number are functions of position along the field s, so we can do a spatial average of the delta function.

In our particle simulation, the field line is divided into grid cells, and potentials, fields, and forces are grid quantities. At one boundary of the cell, the parallel velocity defined by the delta function is $[\Omega(s)-\omega]/k(s)$; at the other, $[\Omega(s+\Delta s)-\omega]/k(s+\Delta s)$. If in the cell, the parallel velocity of the particle is between these two velocities, it diffuses by the waves, otherwise not. Thus, we can replace the delta function with

$$\delta(\omega - kv_z - \Omega) = [k(s)\Delta v_z(s)]^{-1} \; for \left[\frac{\Omega(s)-\omega}{k(s)}\right] > v_z > \left[\frac{\Omega(s+\Delta s)-\omega}{k(s+\Delta s)}\right]$$

$$= 0 \text{ otherwise} \qquad (26)$$

Also, $\Delta v_z(s)$ can be approximated as

$$\Delta v_z(s) = \Delta s \left\{ \frac{\partial}{\partial s} \left(\frac{[\Omega(s) - \omega]}{k(s)} \right) \right\} \qquad (27)$$

This gives rise to a diffusion coefficient D as shown in Fig.(5a) in the solid curve.

We wish here to apply this diffusion to a particle simulation scheme. This means replacing the Fokker-Planck equation with an equivalent Langevin equation as in Ref. 4. Thus in the Langevin equation, in each time step, we add a random addition to v_z. This addition has Gaussian statistics, and whose mean square is $D\delta t$.

One must exercise care in defining the time step δt, because the delta function in Eq.(25), indicates that all quantities are varying rapidly in space and as a function of velocity, and the particle may move quickly through the resonant region. We consider two possible cases. For Case 1, say that the particle does not travel out of the space step Δs in the simulation time step Δt. ($v_z < \Delta s/\Delta t$). Usually this is a required for thermal electrons in a particle simulation. In this case, $\delta t = \Delta t$. On the other hand, for fast electrons with $v_z > \Delta s/\Delta t$, (Case 2), the time the particle undergoes diffusion is given by $\Delta s/v_z$, so $\delta t = \Delta s/v_z$. This is simply the time that the particle is in the grid cell where the diffusion takes place. Then, Δs drops out, so there is no dependence on time or space step in this case. Thus in the case of high velocity particles, the diffusion is characterized by a particle moving through a diffusing region and getting a particular kick in velocity upon crossing the region. This is similar in spirit to the technique of Ashtiani et al[15], and also of our own simulations[2] up to this point. Low velocity particles, by contrast, diffuse within the grid cell in our simulation model. Since the resonant velocity decreases as we approach cyclotron resonance, there will be some position where the resonant velocity is just $\Delta s/\Delta t$. Closer to cyclotron resonance, the particles are Case 1, further out they are Case 2

We now consider the dynamic friction for the parallel motion. This is simply minus the derivative of the diffusion coefficient.

$$F_d = -\partial D/\partial v_z \qquad (28)$$

This is just two delta functions, which might be approximated as in the solid curve of Fig (5b). For numerical reasons it might be simpler to take a smoother function for both, for instance a Gaussian for the diffusion and its derivative for the dynamic friction. These are shown as the dotted curves in Fig.(5). For quasi-linear diffusion, the diffusive change in velocity in a time step, proportional to $E\Delta t^{1/2}$ is much greater than that from the dynamic friction, proportional to $E^2\Delta t$. The dynamic friction would be applied in the normal way in the case of $v_z < \Delta s/\Delta t$. Depending on just what the particle velocity is with respect to the resonant velocity, the force may be either positive or negative. On the other hand, if $v_z > \Delta s/\Delta t$, then the change in velocity from the dynamic friction would be the acceleration times $\Delta s/v_z$. In either case, the change in velocity from the dynamic friction

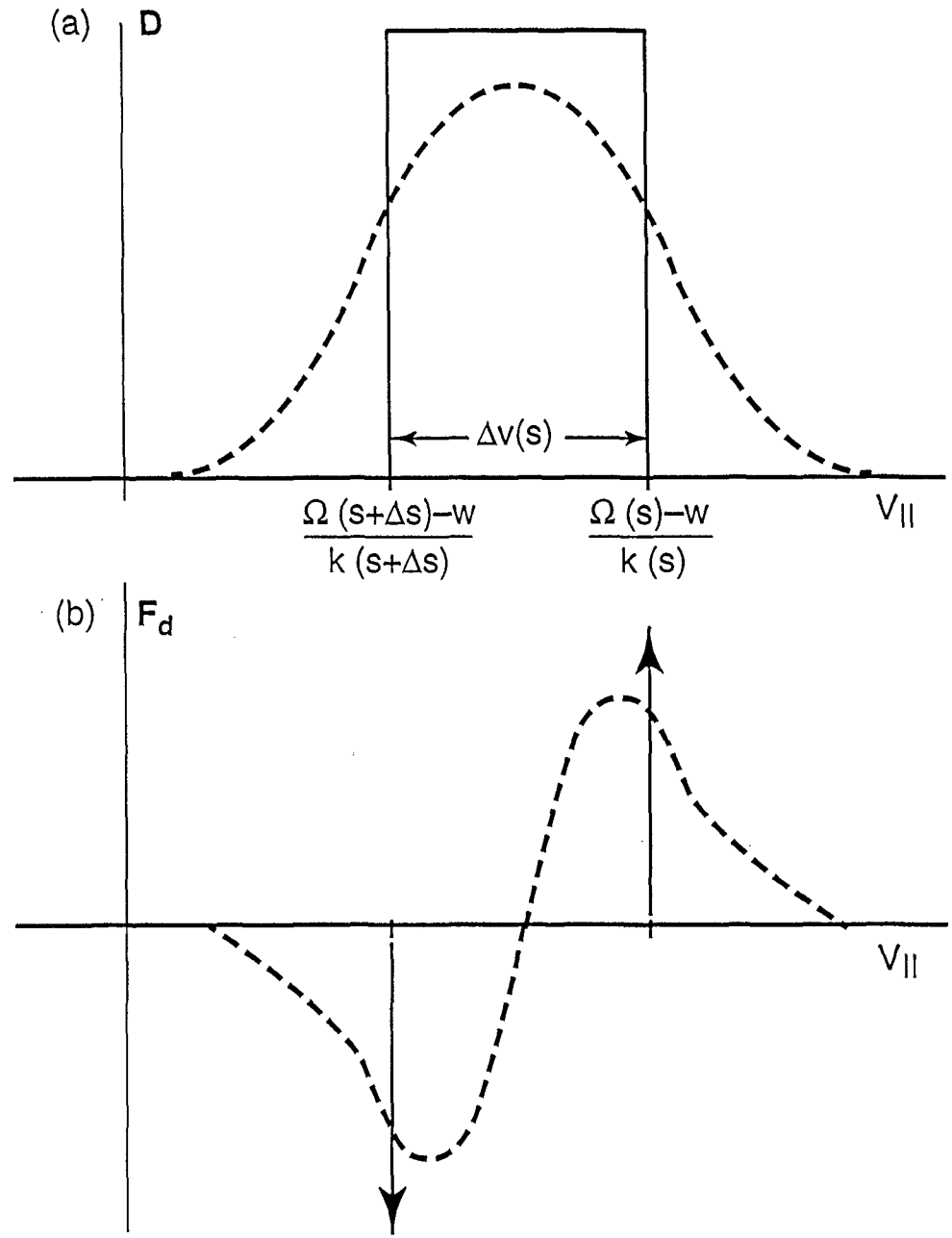

Fig. 5 - Solid, (a) diffusion, and (b), dynamical friction as a function of velocity; and dotted, smoothed out approximations.

might be positive or negative, depending on just what the particle velocity started at. Including the change in velocity as the particle undergoes its various accelerations and diffusions, the orbit itself may average out the positive and negative contributions to the dynamic friction. In either case, the result of the dynamic friction would be to produce small average change in velocity when averaged over all particles.

Once the change in parallel velocity is calculated, the change in perpendicular velocity is calculated by Eq. (24). This then completes the formulation of the absorption of the cyclotron waves and the associated self consistent heating of the electrons.

The only potential difficulty is that the Langevin equation is statistical, whereas the wave kinetic equation is not. Therefore there will be statistical fluctuations to the energy conservation. If necessary, this can be corrected by adding a correction to the velocity of each diffusing electron as was done in the calculation of electron-electron collisions with a Langevin equation[4]. However this is probably not necessary. The particle distribution is calculated correctly within the limits of statistical accuracy; only total energy conservation is not quite correct. If in some period of time, say 500 Watts of microwave power injected, and only 485 watts is absorbed, the error is probably not significant. Alternatively one could simply redefine the microwave power.

VI. Summary

Let us now summarize the steps to the implementation of this scheme. First, at the input waveguide, specify a bundle of rays, all of them having frequency ω and each one having energy density specified by some input profile, perhaps the distribution of power across the face of the input waveguide. The initial perpendicular k is small and may be approximated as zero, or perhaps specified by the waveguide dimensions. Then calculate wave number and the group velocity across the input profile as well. Then for each ray, calculate the ray path. In some cases, it might be reasonable to approximate this ray path as the field line. The next thing is to calculate the cyclotron frequency, along the ray, from the specified magnetic field. Then from the expressions for dispersion relation and group velocity, calculate the wave number, the group velocity and the minimum resonant electron momentum p_m, as a function of position along each ray. Then calculate the damping of the cyclotron wave at each point from Eq.(17) where f(p) is, taken from the electron simulation at the previous time step. If there is not a sufficient number of particles in a grid cell for an accurate calculation of f(p) at each position, it might be necessary to average over several local grid cells, or even the entire field line to get an appropriate f(p). Then integrate for W along each ray (or field line) by solving Eq.(10 A or B). From W(s), calculate $E^2(s)$ from Eq.(6); then use this electric field in the in the expression for the diffusion coefficient and dynamic friction in the Langevin equation for the parallel motion of the electrons. In this way the electron distribution function is advanced in a way self consistently with the absorption of the cyclotron waves. This formulation is valid and self consistent even though the electron distribution might or might not be Maxwellian, and its tail might be depleted or overpopulated due to various competing physical processes. The scheme is simple and numerically efficient, since no new time scales are added to the formulation[2]. The computer time to solve it and the human time to code it up are both minimized.

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